Theories of non-Fermi liquid behavior in heavy fermions.

P. Coleman
Serin Laboratory, Rutgers University, P.O. Box 849, Piscataway, NJ 08855-0849, USA.
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I will review our incomplete understanding of non-Fermi liquid behavior in heavy fermion systems at a quantum critical point. General considerations suggest that critical antiferromagnetic fluctuations do not destroy the Fermi surface by scattering the heavy electrons- but by actually breaking up the internal structure of the heavy fermion. I contrast the weak, and strong-coupling view of the quantum phase transition, emphasizing puzzles and questions that recent experiments raise.

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Although heavy fermion behavior came to light over twenty years ago, we forget that consensus about the Fermi liquid nature of the normal state took nearly a decade to develop. The last five years have seen a new struggle to understand the persistent deviations from Fermi liquid behavior that occur in some of these compounds.[1]

Several aspects of non-Fermi liquid behavior will be discussed at this conference, in particular, the vital effects of disorder and inhomogeniety.[2–4] Here however, I shall focus on a new body of evidence which shows that non-Fermi liquid behavior develops in single-crystal heavy fermion compounds at an antiferromagnetic quantum critical point (Q.C.P). Our understanding of the new metallic state this gives rise to is currently very incomplete and I shall try to emphasize the questions we are posed.

Antiferromagnetic quantum critical behavior occurs in many heavy fermion metals, including $CePd_2Si_2$,[5] $CeIn_3$,[5] $CeNi_2Ge_2$,[6] $CeCu_{6-x}R_x$ ($R = Au,\ Ag$),[7,8] $CeRu_2Si_2$[9] and $U_2Pt_2In_2$.[10] Either by pressure,[11] doping or a magnetic field,[8] these compounds can be reproducibly brought to a QCP where the Neél temperature vanishes. At this point various non-Fermi liquid properties develop, such as

- Anomalous power-law temperature dependence of the resistivity. In $CePd_2Si_2$ for example, a power-law $\rho \propto T^{1.2}$ is seen on both the antiferromagnetic, and the paramagnetic side of the transition.
- Non Curie temperature dependence of the susceptibility.
- Anomalous logarithmic temperature dependence of the specific heat $C_v/T = A\ln(T^*/T)$. In $CeCu_{6-x}R_x$, the same A and T^* are observed at the critical point, no matter how it is approached.[7]

As the quality of the samples improves, the non-Fermi liquid behavior persists, and in the case of $CePd_2Si_2$ and $CeGe_2Ni_2$, superconductivity is found to develop at low temperatures in the vicinity of the QCP.

Doniach[12] first proposed the possibility of dense Kondo behavior in heavy fermion compounds, suggesting that when the ratio of the single ion Kondo temperature T_K to the RKKY interaction scale T_{RKKY} exceeds a critical value, magnetism would vanish. The possibility that the transition might be continuous was not appreciated until recently, and has special significance.[13,14] If we think of local moment antiferromagnetism (AFM) and Fermi liquid (FL) behavior as two competing attractive fixed points of a renormalization group trajectory, then the existence of an antiferromagnetic QCP tells us that these two limits are linked by new fixed point. (Fig. 1). As the

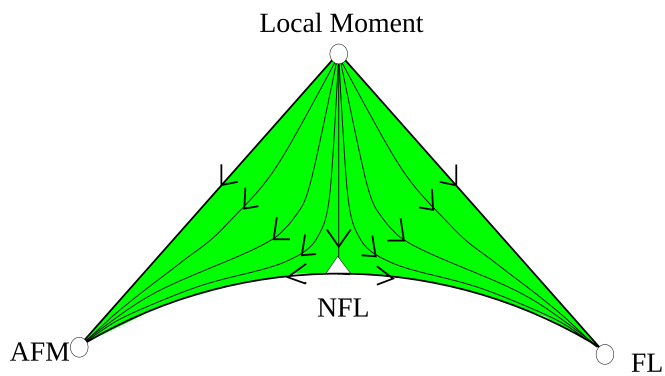

FIG. 1. Schematic scaling diagram for the Kondo Lattice

temperature is lowered, the effective Hamiltonian evolves away from high-temperature local moment behavior to one of two alternate attractive fixed points. By tuning a material, using pressure or some other means, to the critical value of T_K/T_{RKKY}, it is forced to evolve along a separatrix to the QCP. More importantly, a wide range of materials close to this critical value will pass close to the new fixed point, and over a large temperature range their properties, excitations and interactions will be dominated by the physics of this QCP.

A. Weak versus strong-coupling approaches

The scaling diagram tells us that there are two ways of regarding the transition from heavy fermion behavior to antiferromagnetism. A "weak coupling" approach starts

on the Fermi liquid side, and regards the QCP as a magnetic instability of the Fermi surface. The alternative strong coupling approach starts from the magnetic side, and regards these metals as local moment systems which lose their magnetism once the single-ion Kondo temperature is large enough to develop a dense Kondo effect.

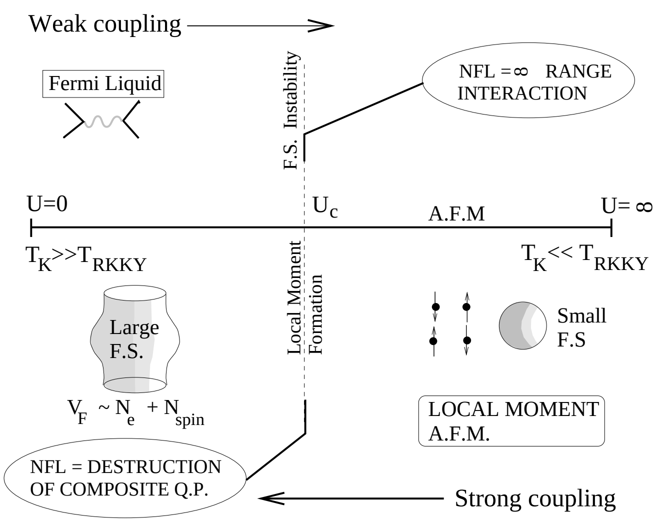

FIG. 2. Contrasting the weak, and strong-coupling picture of an antiferromagnetic QCP.

From the first perspective, the magnetic instability develops in momentum space; non-Fermi liquid behavior is driven by the infinitely long-range and retarded interactions that develop between quasiparticles at the QCP. From the second perspective, quasiparticles in the Fermi liquid are composite bound-states formed in *real space* between local moments and conduction electrons; at the critical point, the bound-states which characterize the Kondo lattice disintegrate to reveal an underlying lattice of ordered magnetic moments. The challenge is to reconcile hese two viewpoints into a single unified picture of the critical magnetic fluid.

B. Weak-coupling Approach

The weak-coupling approach has a long history founded in spin-fluctuation picture of ferromagnetism.[26] More recently, Hertz and Millis[27,28] have recast this approach in a modern renormalization-group language. Hertz made the key observation that at a QCP, the correlation time diverges more rapidly than the correlation length, according to the relation

$$\tau \propto \xi^z, \tag{1}$$

where z is called the dynamical critical exponent. Hertz identified z as an anomalous scaling dimension of time $[\tau] = [x]^z$, raising the effective dimensionality of a QCP from $3 + 1$ to $D = 3 + z$. When $D > 4$, interactions amongst the magnetic modes vanish in the continuum limit, where they behave as Gaussian degrees of freedom. Since spin fluctuation theory predicts $z = 2$ at an antiferromagnetic QCP, a priori, it should provide a perfectly self-consistent description of antiferromagnetic QCP's in three dimensions.

In spin-fluctuation theory, the heavy fermion metal is described by a featureless band of electrons, with Hamiltonian

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^{\dagger}{}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} J(\mathbf{q}) \mathbf{S}_{\mathbf{q}} \cdot \mathbf{S}_{-\mathbf{q}} \tag{2}$$

where $\mathbf{S}_{\mathbf{q}} = \sum_{\mathbf{k}} c^{\dagger}{}_{\mathbf{k}} \boldsymbol{\sigma} c_{\mathbf{k}+\mathbf{q}}$ is the spin density and $J(\mathbf{q})$ the magnetic interaction strength at wavevector $\mathbf{q}$. In an RPA treatment of this model, the dynamical magnetic susceptibility is

$$\chi_{(}\mathbf{q},\omega)^{-1} = \chi_o(\mathbf{q},\omega)^{-1} + J(\mathbf{q}) \tag{3}$$

where χ_o is the bare magnetic susceptibility. When interactions reach a value where, at some critical wavevector $\mathbf{Q}$, $J(\mathbf{Q}) = -\chi_o(\mathbf{Q})^{-1}$, the susceptibility diverges and magnetic order condenses at wavevector $\mathbf{Q}$.

In the weak-coupling picture, at the QCP,

$$\chi_{(}\mathbf{q},\omega)^{-1} = [\delta + a^2(\mathbf{q} - \mathbf{Q})^2 - i\omega/\Gamma]/\chi_o \tag{4}$$

where χ_o is the uniform magnetic susceptibility, a is of order the lattice spacing; δ is a quantity characterizing the distance from the QCP and Γ characterizes the characteristic energy scale of spin fluctuations. From this form, we see that the characteristic spin-correlation length and time are given by

$$\xi \sim \frac{a}{\delta^{\frac{1}{2}}}, \qquad \tau \sim \frac{1}{\Gamma\delta} \tag{5}$$

so that $z = 2$. This is one of the <u>central</u> predictions of the weak-coupling approach. According to the Hertz-Millis theory, in dimensions $d > 4 - z = 2$, it should be possible to regard the magnetic fluctuations as a sort of overdamped exchange boson, propagating a long-range interaction given by

$$V(q) = J(q)^2 \chi(q,\omega) \tag{6}$$

This type of theory provides a remarkably good description of ferromagnetic QCP's that develop in transition metals.[11] Unfortunately, it has become increasingly clear, that it is inadequate for the QCP in heavy fermion metals. In particular:

- The theory predicts that the critical fluctuations will give rise to an anomalous specific heat $\Delta C_V/T \propto T^{(d-z)/z} \sim T^{1/2}$ in three dimensions. In both $CeNi_2Ge_2$[6] and $CeCu_{6-x}Au_x$,[7] a logarithmic temperature dependence of C_V/T is observed.

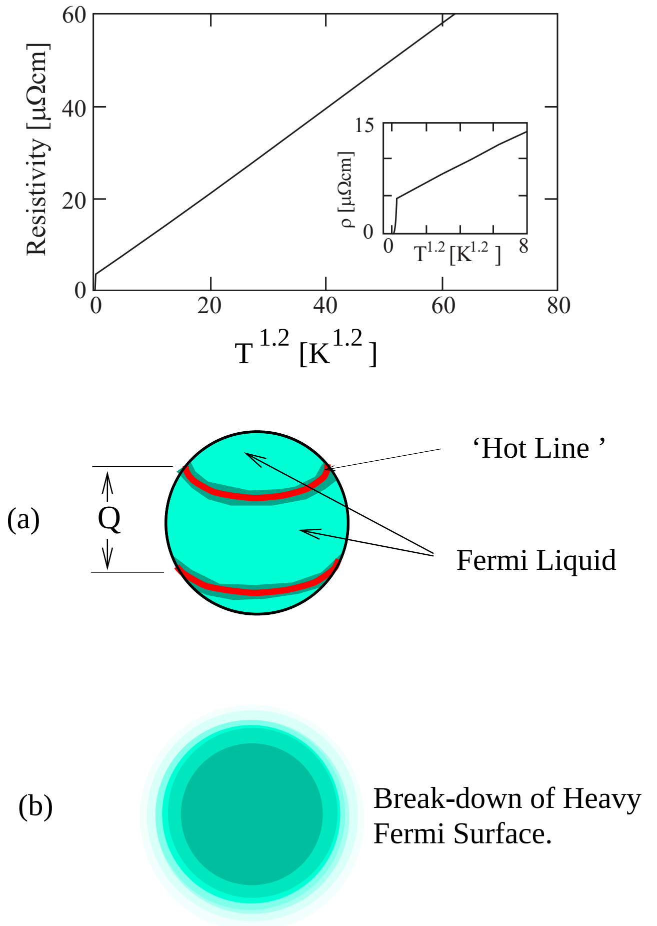

FIG. 3. Anomalous resistivity of $CePd_2Si_2$ at the critical pressure, after Julian et al. (a) In the simplest spin-fluctuation picture, magnetic scattering leads to "hot lines" around the Fermi surface, separated by regions of normal Fermi liquid which would short-circuit the conductivity at low temperatures (b) The absence of any T^2 regime in the resistivity suggests that sharply defined quasiparticles are eradicated from the entire heavy Fermi surface.

- The theory does not lead to a break-down of Fermi liquid behavior, in the strict sense that the quasiparticles are well defined on most of the Fermi surface, excepting in the vicinity of the "hot lines" that are linked by the magnetic $\mathbf{Q}$ vector on the Fermi surface (3). On the hot lines, the quasiparticle scattering rate $\Gamma_{\mathbf{k}} \propto \sqrt{T}$, but away from the hot lines, the quasiparticle scattering rate has the classic Fermi liquid form $\Gamma_{\mathbf{k}} \propto T^2$.[15]

This last point was first noted by Hlubina and Rice,[15] but is still not widely appreciated. The presence of large regions of normal Fermi surface between the hot lines implies that at temperatures below the spin-fluctuation scale Γ_o, the cold regions of the Fermi surface will short-circuit the conductivity to produce a T^2 resistivity. Such a cross-over to Fermi liquid behavior has never been seen.

These difficulties prompted the Karlsruhe group to carry out a detailed neutron scattering study of $CeCu_{6-x}Au_x$ at the critical doping $x = 0.1$. Early measurements showed that the spin fluctuation spectrum is peaked along *rods* in momentum space, rather than around a single Bragg peak[16,17]. This led Rosch et al. to propose that, the magnetic fluctuations in this material are quasi-two dimensional. This hypothesis very elegantly deals with the two difficulties mentioned above, for once $d = 2$, the predicted specific heat becomes logarithmic; furthermore, the absence of any well defined scattering wavevector along the length of the magnetic rods, implies that the hot-rings are smeared out over a broad region of the Fermi surface, partially eliminating the second criticism. The development of spin fluctuations of reduced dimensionality in a fully three-dimensional crystal is already a very serious departure from our expectations. Even this is not enough to save the weak coupling picture, as I now discuss.

C. Strong-coupling Approach

What could possibly go wrong with the weak-coupling spin fluctuation theory? One potential shortcoming is that it fails to account for the essentially local physics of the Kondo effect and moment formation. More that two decades ago, Larkin and Melnikov[18] pointed out that the Kondo effect can break down at a QCP. These authors found that if a local moment is immersed in a conduction sea at a Ferromagnetic QCP, the conventional Kondo effect does not take place; instead, the local moment forms a bound-state with the magnetic lattice in an effect which does not depend on the sign of the coupling.

Were the Kondo effect to fail at an antiferromagnetic QCP, then the entire strong-coupling picture of the antiferromagnetic QCP would change. At present, there is no theory for the Kondo effect at an antiferromagnetic QCP. However,the break-down of the Kondo effect at a QCP has been considered in other contexts[19], particularly that of quantum spin-glasses.[20–22] A common thread to these theories is the idea that if the local moment becomes critically screened at the QCP, the spin correlations will develop power-law correlations in time, up to cut-off times of order $\hbar/k_BT$. This would then lead to ω/T scaling in the spin-susceptibility

$$\chi(\omega, T) = \frac{1}{T^\alpha} f(\frac{\omega}{T}) \tag{7}$$

This kind of behavior is not generally expected in Hertz-Millis theory, but apparently, it *is* observed in heavy fermion systems. ω/T scaling was first observed in neutron scattering experiments on powder samples of UCu_4Pd, which is believed to lie close to a magnetic QCP.[19] More recently, ω/T scaling was observed at the critical wavevector in $CeCu_{5.9}Au_{0.1}$[23], where the measured magnetic susceptibility can be fitted by a form

$$\chi(\mathbf{q}, \omega)^{-1} = [J(\mathbf{q}) + a(-i\omega + T)^\alpha], \quad (\alpha = 0.8) \tag{8}$$

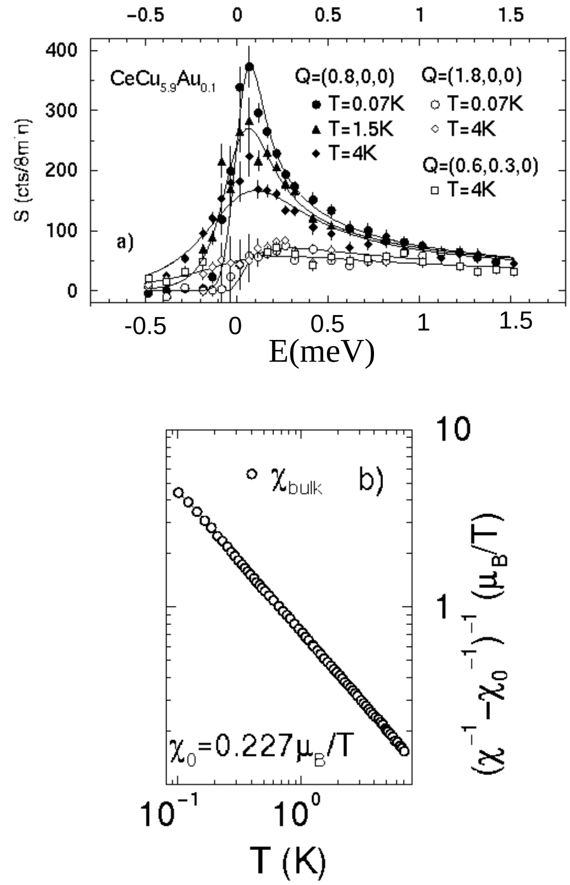

FIG. 4. ω/T scaling is manifested in the inelastic neutron scattering from $CeCu_{6-x}Au_x$, and the very same scaling exponent is found in the uniform suscepibtility.

At the critical wave-vector $\mathbf{q} = \mathbf{Q}$, $J(\mathbf{Q}) = 0$ vanishes, and (8) becomes identical to (7). Remarkably, the same exponent $\alpha = 0.8$ appears to dominate the *entire* Brillouin zone, and re-appears in the uniform susceptibility, which can be fitted to a form $\chi(T)^{-1} = (J(0) + aT^{0.8})$ (Fig. 4) . It follows that the dynamical critical exponent is $2/\alpha = 2.5$- a serious departure from the weak-coupling picture.

Sengupta has suggested a simple way to think about this type of behavior, proposing that when the Kondo effect breaks down, the Weiss field $\vec{h}$ acting on the local moments develops critical correlations in time,

$$\langle h_a(\tau) h_b(\tau')\rangle \sim \frac{\delta_{ab}}{(\tau - \tau')^{2-\epsilon}} \tag{9}$$

Any value of $\epsilon > 0$ represents a strong departure from Fermi liquid behavior. To see that kind of behavior is consistent with the magnetic correlations observed in $CeCu_{6-x}Au_x$, let us relate the Weiss field to the spin density by writing $h(q) = J(q)S(q)$. It follows that the Weiss-field correlation function is

$$\langle h^a(\mathbf{q}, \omega) h^b(-\mathbf{q}, -\omega)\rangle = J(\mathbf{q})^2 \chi^{ab}(\mathbf{q}, \omega) \tag{10}$$

But if we use the form (8), the local correlation function of the Weiss-field is given by

$$\begin{aligned}\langle h^a(\omega) h^b(-\omega)\rangle &= \delta^{ab} \int \frac{d^3q}{(2\pi)^3} \frac{J(\mathbf{q})^2}{J(\mathbf{q}) + a(-i\omega + T)^\alpha} \\ &\propto (-i\omega + T)^\alpha + \text{cons}\end{aligned} \tag{11}$$

where the zero $J(\mathbf{Q}) = 0$ suppresses the singular contribution around $\mathbf{q} = \mathbf{Q}$. But if $\mathrm{Im}\langle h^a(\omega) h^b(-\omega)\rangle \sim \omega^\alpha$, it follows that $\langle h^a(t) h^b(0)\rangle \sim 1/t^{1+\alpha}$, showing that $\epsilon = 1 - \alpha = 0.2$ in $CeCu_{6-x}Au_x$. Notice incidentally that in spin-fluctuation theory $\alpha = 1$, so $\epsilon = 0$ and the Weiss field shows no departure from Fermi liquid behavior.

Inspired by early work of Sachdev and Ye on quantum spin-glasses[20], Sengupta[21] has argued that the effective action of a local moment subjected to this fluctuating field in a cavity should take the form

$$I = \int_0^\beta d\tau d\tau' S^a(\tau) \langle h_a(\tau) h_b(\tau')\rangle S^b(\tau'), \tag{12}$$

At certain stable values of ϵ, the spins must develop powerlaw correlations in such a way that the action is scale-invariant. Since the scaling dimension of $[h] = \tau^{-1+\epsilon/2}$, it follows that $[S] = \tau^{-\epsilon/2}$, so that $\langle S(\tau)S(0)\rangle \sim \tau^{-\epsilon}$, corresponding to a cavity spin susceptibility $\chi_o(\omega)^{-1} \sim (-i\omega)^{1-\epsilon}$. When we couple the cavity up to its environment,[24] we obtain

$$\chi(\mathbf{q}, \omega)^{-1} = (\chi_o(\omega)^{-1} + J(\mathbf{q})), \tag{13}$$

which recovers the phenomenological form (8) observed in experiment. Unfortunately, although these arguements establish the stability of a QCP with Weiss fields that are critically correlated in time, they provide no insight into its microscopic origins, in particular: (i) the observed value of ϵ, (ii) the detailed momentum dependence of the magnetic fluctuations, and (iii) how the critical magnetic fluctuations couple to, and scatter electrons.

D. More mysteries indicate the need for new microscopic theory.

It turns out, as Stockert will discuss at length, that the soft spin-fluctuations at the QCP actually occupy a "dog-bone" shaped (>—<) region of momentum space, rather than a simple tube as first supposed.[17,23] This is reminiscent of a frustrated magnet lying close to an incommensurate- commensurate phase transition, or Lifschitz point. This led us[23] to propose that in the vicinity of the magnetic Bragg peak, the spin-stiffness becomes quartic in momentum in directions parallel to the arms of the "X"-shaped scattering maximum, i.e. $J(\mathbf{q}) \sim A\delta q_\perp^2 + B\delta q_\parallel^4$. In the Free energy, the soft directions provide less phase space for fluctuations and only count as one half-dimension, so the effective dimensionality for the thermodynamics is $D_{eff} = 2 + \frac{1}{2}$ Curiously, this exactly matches the dynamical critical exponent $z = 2.5$ deduced from the neutron scattering, so that

a logarithmic specific heat is predicted by the theory, but now the hot-line problem returns.

In this paper I have tried to argue that the observation of

- critical fluctuations in the Weiss field.
- Reduced dimensionality of the magnetic fluctuations.
- Non-trivial exponents in the resistance

demand a new approach to the physics of the antiferromagnetic QCP in heavy fermion systems, possibly one that incorporates the physics of moment formation and the Kondo effect. What sort of features might we expect in such a theory? Let me make a few speculative remarks to stimulate discussion. One of the weak central assumptions of spin-fluctuation theory, is that the amplitude vertex for the process

$$e^-_{\mathbf{k}\uparrow} \rightleftharpoons e^-_{\mathbf{k}-\mathbf{Q}\downarrow} + \text{spin-fluctuation} \tag{14}$$

is non-singular at the QCP. If indeed the Kondo effect fails at a QCP, it is tempting to suggest that this assumption must fail. How? Clearly we need to think about how the composite heavy electron, itself a bound-state between electrons and local moments, decays. To obtain a singular decay process, perhaps one needs some kind of local excitation, giving rise to a process of the following form

$$\mathrm{f}_{\mathbf{k}\sigma} \rightleftharpoons \mathrm{b}_{\mathbf{k}'\sigma} + \Phi \tag{15}$$

where $\mathrm{f}_{\mathbf{k}\sigma}$ represents the composite heavy electron formed as part of the Kondo effect, $\mathrm{b}_{\mathbf{k}'\sigma}$ represents the magnetic excitation, written here in the language of Schwinger bosons, and Φ is a massless fermionic excitation (charged, yet spinless) that has no overlap with the heavy quasiparticle states, which plays a role in mediating the interaction between heavy fermions and paramagnons. Such a hypothetical excitation is motivated by the observation of a powerlaw spin correlation that dominates the entire Brillouin zone; it would also provide a mechanism to destroy the Fermi surface uniformly, rather than along hot-lines. This kind of structure may develop in "supersymmetric" approaches to the Kondo lattice problem, which describe the local moments by a partner of bosonic and fermionic degress of freedom.[29,30]

Putting speculations aside, there is clearly strong motivation to extend the sort of measurements made on $CeCu_{6-x}Au_x$ to stoichiometric compounds, such as $CeGe_2Ni_2$, to establish whether critical Weiss fields are a pervasive feature of the heavy fermion QCP. On the theoretical front, there is evidently a desperate need for us to re-examine the whole issue of how the local moment starts to reveal itself at quantum criticality.

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